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NIST
PUBLICATIONS

NIST STANDARD REFERENCE DATA PRODUCTS 1990 CATALOG

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NIST Special Publication 782

NIST Standard Reference Data Products 1990 Catalog

Malcolm W. Chase, Jr., Editor

Standard Reference Data
National Institute of Standards and Technology
Gaithersburg, MD 20899

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ABSTRACT AND KEY WORDS

The National Institute of Standards and Technology's Standard Reference Data Program provides reliable, well-documented data to scientists and engineers for use in technical problem-solving, research, and development. This catalog lists classic data compilations in hard-copy form and current databases in the Standard Reference Database Series. These data compilations have been subdivided into seven categories. Prices and ordering information are located at the back of the document.

Key words: atomic physics; chemistry; compilations; database; materials; numeric data

PREFACE

As a result of the Omnibus Trade and Competitiveness Act, signed into law on August 23, 1988, the National Bureau of Standards officially became the National Institute of Standards and Technology (NIST). The new institute retains all of the traditional functions and services of NBS and takes on several new assignments designed to boost American industry in the world marketplace. NIST is working with several new constituencies, including state and local economic development organizations. Existing NBS programs are continuing under NIST. Four major new programs are mandated by the legislation: the development of regional centers for transfer of manufacturing technology; the creation of a focal point within the Federal Government to work with and support state and local industrial extension services; the creation of an advanced technology program to support and encourage the rapid commercialization of promising new inventions and technologies; and the creation of a national clearinghouse of information on state and local technology development initiatives.

The formal existence of the NSRDS dates from 1963, when the Federal Council for Science and Technology asked the National Bureau of Standards to assume primary responsibility in the Federal Government for promoting and coordinating the critical evaluation of numerical data in the physical sciences. The program was conceived as a decentralized national effort with financial support coming from a variety of Government and private sources, but with NBS responsible for all the overall planning and coordination. In 1968, Congress provided a specific legislative mandate for the program through passage of Public Law 90-396, the Standard Reference Data Act. This Act states the policy of Congress to make reliable reference data available to scientists, engineers, and the general public.

The Standard Reference Data Program has been providing evaluated, high-quality data for a wide range of applications to industry, government, and academic institutions for over 20 years. Standard reference data have been utilized to improve design efficiency of various chemical processes, identify potentially toxic substances in the environment, improve materials durability, and calculate performance of chemical reactors, to name but a few applications. With the onset of the personal computer, standard reference data are even more accessible and will play an even more critical role in the future.

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INTRODUCTION

The NIST Standard Reference Data (SRD) Program provides reliable, well-documented data to scientists and engineers for use in technical problem-solving, research, and development.

Experts in the physical, chemical, and materials sciences critically evaluate data that result from experimental measurements, calculations, and theory. The evaluations are carried out through a network of data centers, projects, and cooperative programs that comprise the National Standard Reference Data System (NSRDS). Experienced researchers in each area assess the accuracy of the data reported in the literature, prepare compilations, and recommend best values. The outputs are widely distributed as publications and computer-readable databases.

LEFT: *The Standard Reference Data Management Group (standing l to r) Eugene S. Domalski, Manager, Chemical Data; John R. Rumble, Manager, Materials Data; (seated l to r) Jean W. Gallagher, Manager, Physical Data; and Malcolm W. Chase, Jr., Acting Chief, Standard Reference Data.*

BELOW: *The administrative staff of SRD consists of (standing l to r) Diane Frizzell, Joan Sauerwein; (seated l to r) Pat Kurak, Margaret Bradley, and Jeanne Bride. Not pictured are Cheryl Williams, Debbie Justus, and Alice Dugan.*

The formal existence of the SRD Program dates from 1963, when the Federal Council for Science and Technology asked the then-National Bureau of Standards to assume primary responsibility for coordinating the critical evaluation of numerical data in the physical sciences. In 1968, Congress provided specific legislation for the program through passage of the Standard Reference Data Act (PL 90-396).

Current activities in the Standard Reference Data Program are carried out in long-term data centers, located primarily at NIST, and numerous short-term projects, primarily at university and industrial research centers. In addition, the Program maintains many long-term collaborations with industry on cooperative data programs which draw support from industry and government.

The activities concentrate on the disciplines as follows:

Analytical Chemistry —includes mass spectral data, surface analysis data, and crystallographic data for chemical identification.

Atomic Physics —includes atomic energy levels, transition probabilities, and collision data used for characterization and modeling.

Chemical Kinetics —includes evaluated data on gas-phase reactions.

Materials Properties —structure and characterization of materials, performance properties, including corrosion and phase equilibria.

Molecular Structure and Spectroscopy —evaluated data on molecular structures and microwave spectra.

Thermochemistry —includes reliable, widely-used tables of organic and inorganic species.

Thermophysical Properties of Fluids —thermophysical properties of pure and mixed fluids that are of great importance to industry.

Dissemination vehicles are as follows:

National Standard Reference Database Series—Databases on diskettes, magnetic tapes, and online systems

Journal of Physical and Chemical Reference Data—A bimonthly journal published jointly with the American Chemical Society and the American Institute of Physics

NIST Publication Series—Various technical report series published by NIST

Other joint publications—Journal and books published with technical society and private publishers

Dr. David R. Lide, Editor of the Journal of Physical and Chemical Reference Data.

When ordering an SRD database, checks, purchase orders, Visa, and Mastercard are accepted. Orders can be placed by phone or FAX for quick turn-around. For further information on SRD databases, please contact:

Joan Sauerwein
Standard Reference Data
National Institute of Standards and Technology
Bldg. 221/Room A323
Gaithersburg, MD 20899
(301)975-2208
(301)975-2183(FAX)

STANDARD REFERENCE DATABASES

1. NIST/EPA/MSDC Mass Spectral

1A. NIST/EPA/MSDC Mass Spectral: PC Version

2. NIST Chemical Thermodynamics

3. NIST Crystal Data Identification

4. NIST Thermophysical Properties of Hydrocarbon Mixtures

7. NIST Electron and Positron Stopping Powers of Materials

8. NIST X-ray and Gamma-ray Attenuation Coefficients and Cross Sections

9. NIST Activity and Osmotic Coefficients of Aqueous Electrolyte Solutions

10. NIST Thermophysical Properties of Water

11. DIPPR Data Compilation of Pure Compound Properties

11A. Student DIPPR

12. NIST Thermophysical Properties of Fluids

The SRD Data Systems Development Group (l to r) Shari Young, Mary Trapane, Phoebe Fagan, and Dorothy Bickham develop and program SRD databases. Not pictured is Gerry Dalton.

13. NIST JANAF Thermochemical Tables

14. NIST Mixture Property Program

15. NIST/Sandia/ICDD Electron Diffraction

16. NIST Corrosion Performance

17. NIST Chemical Kinetics

19A&B. NIST Positive and Negative Ion Energetics

20. NIST X-ray Photoelectron Spectroscopy

21. NIST/CARB Biological Macromolecule Crystallization

23. NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures

24. NIST Atomic Transition Probabilities

26. NIST Vibrational Electronic Energy Levels of Small Polyatomic Molecules

Judy Calabrese (l) and Connie Seymour of the Bedford Composition Group are electronic typesetters for the Journal of Physical and Chemical Reference Data and other SRD publications.

ANALYTICAL CHEMISTRY

In the field of analytical chemistry, the SRD Program provides a set of comprehensive, easy-to-use databases and printed data compilations that help the analytical chemist identify unknown materials, and in many cases, once identified, avoid the need to recharacterize a substance. SRD databases cover a full range of analytical techniques, including mass spectrometry, surface analysis, and crystallographic structure.

To reach the greatest possible audience, the data collections are offered in several formats: as PC diskettes, on magnetic tape for inclusion in in-house laboratory systems, as incorporated into instruments themselves, and via online database systems.

In every case, the data have been fully evaluated, using a variety of techniques. When appropriate, duplicate measurements have been included for completeness. All the databases are updated on a regular basis. The PC diskette version of these databases includes an easy-to-use interface that can be mastered quickly and without having to resort to large manuals.

SRD Analytical Chemistry Databases

NIST/EPA/MSDC Mass Spectral Database
NIST Crystal Data Identification File
NIST/Sandia/ICDD Electron Diffraction Database
NIST X-ray Photoelectron Spectroscopy Database
NIST/CARB Biological Macromolecule Crystallization Database

SRD Major Publications in Analytical Chemistry

Gas-Phase Ion and Neutral Thermochemistry
The Wiley/NBS Registry of Mass Spectral Data (7 vols.)
Crystal Data Determinative Tables (6 vols.)
Elemental and Interplanar Spacing Index

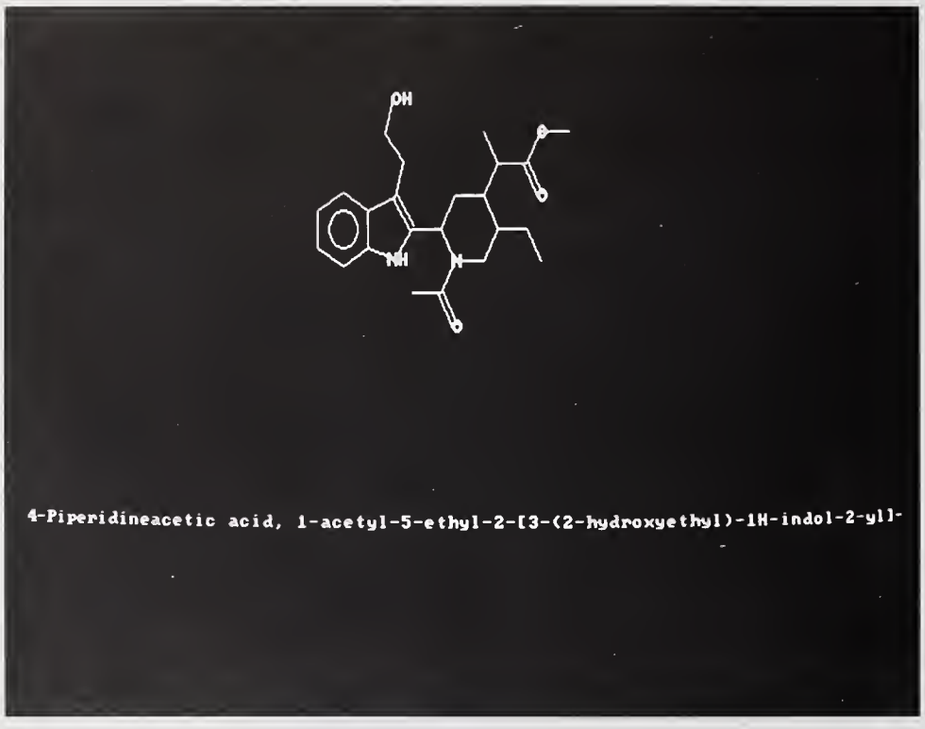
ANALYTICAL CHEMISTRY DATABASES

1. NIST/EPA/MSDC Mass Spectral Database

Sharon G. Lias
Mass Spectrometry Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301)975-2562

The NIST/EPA/MSDC Mass Spectral Database has been assembled from a variety of sources in a joint program of the Environmental Protection Agency, the National Institutes of Health, the United Kingdom Mass Spectrometry Data Center, and the National Institute of Standards and Technology.

The database contains ionization mass spectra of 50,000 different compounds. Each spectrum has a "quality index" associated with it, the Chemical Abstracts Service (CAS) name, synonyms, the molecular weight and formula, and the CAS Registry Number. Structures have recently been included for 85 percent of the spectra. Categories of substances identified are steroids, alkaloids, drugs, derivatives, amino acids, metals, carbohydrates, fatty acids and lipids, pesticides, and primary pollutants.



Structures have been added for 85% of the spectra in the NIST/EPA/MSDC Mass Spectral Database.

This database is available as a magnetic tape, both in ASCII and standard IBM unformatted FORTRAN G. It is also available online nationally and internationally.

1A. NIST/EPA/MSDC Mass Spectral Database: PC Version 2.0

Stephen E. Stein
Mass Spectrometry Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301)975-2505

The PC Version of this database was released in September 1987; Version 2.0 released in December 1988. The PC Version consists of the database of 50,000 electron ionization mass spectra, various index files for rapid data retrieval, and related software for searching the database in various ways. The database can be searched by:

- identification number
- CAS Registry Number
- chemical name
- molecular formula—can also specify up to 10 peaks
- molecular weight—can also specify partial elemental composition up to 10 peaks
- major peaks
  - –more than one set of ordered peaks
  - –molecular weight
  - –elements in the unknown
  - –all elements possibly in the unknown
  - –numbers of atoms of each element
  - –up to 10 peaks with abundance ranges

Dr. Stephen E. Stein, Technical Director of the Mass Spectrometry Data Center, displays masses of peaks in the NIST/EPA/MSDC Mass Spectral Database.

Version 2.0 has many new searching features:

- complete sequential search and research of the entire database
- individual peaks
- automatic searching
- command line options

Another new feature is the utility to add the user's own spectra to the database.

The PC Version of this database is available in AT and PS2 versions.

3. NIST Crystal Data Identification File

Alan D. Mighell
Crystal Data and Electron Diffraction Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301)975-6254

This file contains crystallographic information useful to characterize more than 130,000 inorganic and organic crystalline materials. The data include the reduced cell parameters, reduced cell volume, space group number and symbol, the calculated density, classification by chemical type, chemical formula, and chemical name. Each entry has an associated literature reference.

The database can be utilized as a practical analytical tool for compound characterization and identification because the reduced cell (i.e., the lattice) is unique for most compounds. The database can also be utilized to prevent redeterminations of published structures. In addition, it is useful in conjunction with other data for materials characterization.

The file includes reliable data across the entire spectrum of the solid state including inorganics, organics, minerals, intermetallics, metals, alloys, drugs, antibiotics, and pesticides. Search software, NBS*LATTICE, is provided with the database. The search software provides symmetry and pseudosymmetry determinations, subcell and supercell calculations done systematically, cell transformations, matrix inversions, and identification via lattice matching.

This database is available in magnetic tape and CD ROM formats and is available internationally online. For further information, please contact International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081.

Drs. Vicky Himes and Alan Mighell evaluate new data entries in the NIST Crystal Database.

15. NIST/Sandia/ICDD Electron Diffraction Database

Alan D. Mighell
Crystal Data and Electron Diffraction Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301)975-6254

This database is designed for phase characterization obtained by electron, neutron, or x-ray diffraction methods. The database and associated software permit highly selective identification procedures for microscopic, as well as macroscopic, crystalline materials. The database contains chemical, physical, and crystallographic information on a wide variety of materials (over 70,000) including minerals, metals, intermetallics, and general inorganic compounds.

The Electron Diffraction Database has been designed to include all the data required to identify materials using computerized d-spacing/formula matching techniques. The data for each entry include the conventional cell, reduced cell, lattice type, space group, calculated or observed d-spacings, chemical name, chemical and empirical formula, material class indicators, references, and other parameters.

This database is available in magnetic tape format and in CD ROM format. For further information, please contact International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081.

20. NIST X-ray Photoelectron Spectroscopy Database

Cedric Powell
Surface Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301)975-2534

The NIST X-ray Photoelectron Spectroscopy (XPS) Database gives easy access to photoelectron and Auger spectral data. The database contains over 13,000 line positions, chemical shifts, and splittings resulting from a critical evaluation by Dr. Charles Wagner of the published literature through 1985. The user may search by element, line type, line energy, and many other variables. Users can easily identify unknown measured lines by matching to all previous measurements.

Each record on the database contains:

- Element and chemical compound, including names and formulas
- Line type-photoelectron, Auger, Auger parameter, chemical shift, doublet splitting, other splittings
- Line energy or energy difference
- Experimental details such as calibration, charge reference, and physical state
- Reference citation

This database is available in PC diskette format.

21. NIST/CARB Biological Macromolecule Crystallization Database

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Rockville, MD 20850
(301)251-2244

The NIST/Center for Applied Research in Biotechnology (CARB) Crystallization Database contains crystallization conditions and unit-cell parameters of crystals of biological macromolecules which have been reported in the literature. The biological macromolecules include proteins, nucleic acids, protein:protein complexes, nucleic acid:nucleic acid complexes, protein:nucleic acid complexes, and viruses. This database will provide a convenient method for verification that a particular biological macromolecule has been crystallized, and provide details for reproducing the crystallization procedure.

The general information compiled for each macromolecule includes the name(s), molecular weight, sub-unit composition, and the presence of prosthetic group(s).

The description of the crystallization procedures consists of the macromolecular concentration, temperature, pH, and growth time. If there are unique aspects to the crystallization procedure, they are described in detail. The crystal data include the space group, unit cell dimensions, Z, crystal density, crystal habit, and size.

This database is available in PC diskette format.

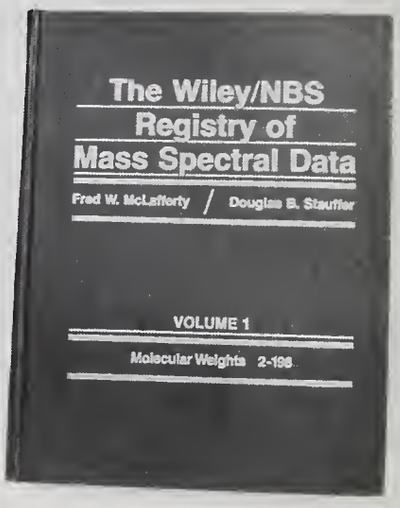
ANALYTICAL CHEMISTRY PUBLICATIONS

Gas-Phase Ion and Neutral Thermochemistry—S.G. Lias, J.E. Bartmess, J.L. Holmes, R.D. Levin, J.F. Liebman, and W.G. Mallard. Journal of Physical and Chemical Reference Data **17**, Supplement 1, 1988.

This volume includes evaluated ionization energies of 4,000 atoms and molecules and proton affinities of 1,000 compounds, as well as electron affinities and gas-phase acidities of approximately 3,000 species. The thermochemistry of the related neutral species is also provided.
Available from the American Chemical Society
US and Canada $70.00
Abroad $84.00

The Wiley/NBS Registry of Mass Spectral Data—F. McLafferty and D.B. Stauffer. Wiley-Interscience, New York, 1988.

This 7-volume work combines mass spectra from the NIST/EPA/MSDC Mass Spectral Database and Wiley's Registry of Mass Spectral Data. Includes spectra of over 112,275 compounds, with structures for over 89,903 compounds. Substance names (CAS and common), molecular weights, empirical formula, and CAS Registry Numbers are provided. Spectra are arranged by ascending molecular weight, elemental composition, and type of compounds. In addition, complete indexing is given.
Available from Wiley-Interscience, New York. $700.00 (set price)



Crystal Data Determinative Tables, Third Edition—6 vols., International Centre for Diffraction Data, Swarthmore, PA.

The NIST Crystal Data Determinative Tables are the largest collection of crystallographic data available. These volumes contain data on over 43,000 organic and organometallic compounds, as well as 27,000 inorganic, metallic, and mineral compounds. Produced and edited by the NIST Crystal Data Center, these reference books are well-indexed by crystallographic system and determinative number. The comprehensive data for each entry include cell dimensions, space group or diffraction aspect, measured and calculated density, name, and literature reference.
Available from the International Centre for Diffraction Data, Swarthmore, PA

Elemental and Interplanar Spacing Index—International Centre for Diffraction Data, Swarthmore, PA.

The Elemental and Interplanar Spacing Index (EISI) is designed to be used independently or in conjunction with a computer database for phase characterization using electron or X-ray diffraction. The EISI is arranged to enable the diffractionist to readily identify a material with the chemical and diffraction data routinely collected on most modern electron column instruments.
Available from the International Centre for Diffraction Data, Swarthmore, PA

ATOMIC PHYSICS

The Standard Reference Data Program has worked together with the world-famous NIST Atomic Physics Program to produce the most comprehensive set of reliable atomic data available anywhere. The NIST collection of atomic energy levels, transition probabilities, and collision data is widely used by groups for characterizing and modeling all types of atomic systems, including plasmas, planetary atmospheres, and astrophysical media, and for health physics applications. Databases and publications make these data easy to find and use.

In recent years, two important databases, one on electron and positron stopping powers and one on x-ray and gamma-ray attenuation, have become widely used. The NIST-published collections of atomic energy levels, transition probabilities, and collisions are being converted into PC databases.

The SRD Atomic Data Program also is responsible for work on revision of the fundamental constants including release of the latest revision in 1986.

SRD Atomic Databases

NIST Electron and Positron Stopping Powers of Materials
NIST X-ray and Gamma-ray Cross Section and Attenuation Coefficients
NIST Atomic Transition Probabilities Data Files (Scandium through Nickel)

SRD Major Publications in Atomic Data

Atomic Transition Probabilities
Atomic Energy Levels Publications
1986 CODATA Recommended Values of the Fundamental Physical Constants

7. NIST Electron and Positron Stopping Powers of Materials

S.M. Seltzer
Photon and Charged Particle Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301)975-5550

The NIST Database on Electron and Positron Stopping Powers and Ranges provides rapid calculation of stopping powers (collisional, radiative, and total), CSDA ranges, radiation yields and density effect corrections for incident electrons or positrons with kinetic energies from 1 keV to 10 GeV, and for any chemically defined target material. The interactive program allows the user to specify incident particle, energy list, target material and density, and for a gas, temperature and pressure. Liberal help screens clearly describe the calculations. Results can be saved to an external file for future use.

This database is available in PC diskette format. A similar database available on magnetic tape extracts comparable information for specific materials (285 for incident electrons and 29 for positrons).

8. NIST X-ray and Gamma-ray Cross Section and Attenuation Coefficients

S.M. Seltzer
Photon and Charged Particle Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301)975-5550

This database (called XGAM) provides photon cross sections (interaction coefficients) and attenuation coefficients for any substance. Interactive software is provided which enables the user to obtain data by entering chemical formulas or other measures of composition for a mixture of component materials. The user may also select the energy range over which data are desired.

The system operates from a database of cross sections for coherent and incoherent scattering, photoionization, and pair production for the elements $Z = 1$ to 100 at energies from 1 keV to 100 GeV. The data supplied were obtained by a critical data analysis combining theoretical and experimental results.

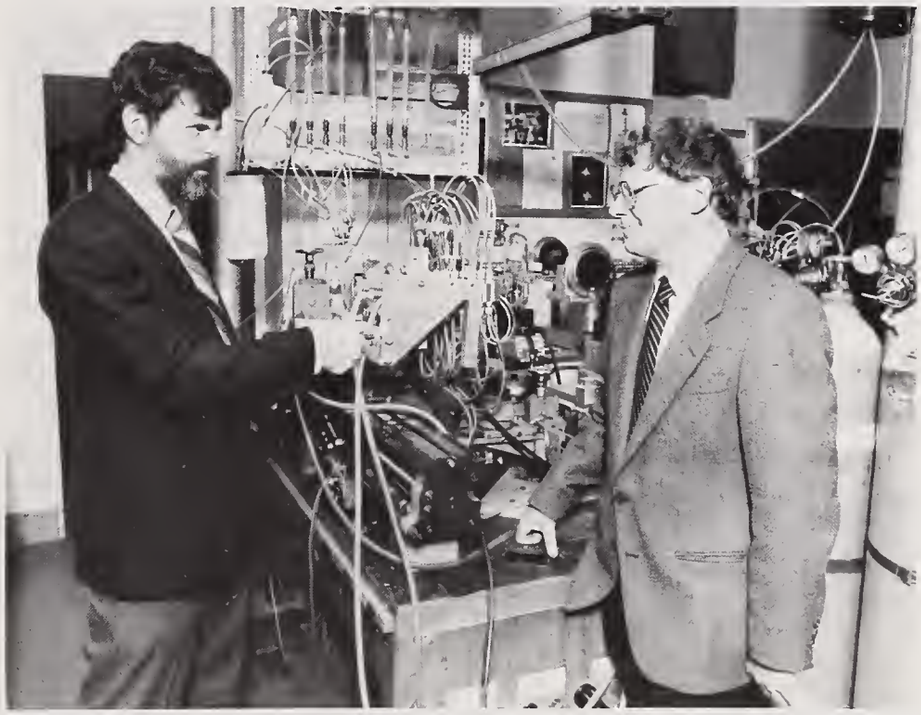
The user may request data to be tabulated at the fixed energies stored in the database, at these fixed energies plus others specified by the user, or at a completely arbitrary set of specified energies. The tabulated results include the individual contributions and the total mass attenuation coefficient, with and without coherent scattering.

This database is available on both a PC diskette and a magnetic tape.

24. NIST Atomic Transition Probabilities Data Files (Scandium through Nickel)

Jeffrey Fuhr
Atomic Transition Probabilities Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301)975-3204

This diskette package provides the numerical data given in "Atomic Transition Probabilities, Scandium Through Manganese" and "Atomic Transition Probabilities, Iron Through Nickel," which were published as Supplements 3 and 4 to Volume 17 (1988) of the Journal of Physical and Chemical Reference Data. The diskettes contain two types of files: the numeric files containing the transition probabilities and related data and the files of references pertaining to the numeric tables. There are eight numeric file names for the elements scandium through nickel and eight reference files, likewise named for these elements and stored separately. Within each element, the data files are ordered by the ionization stage.

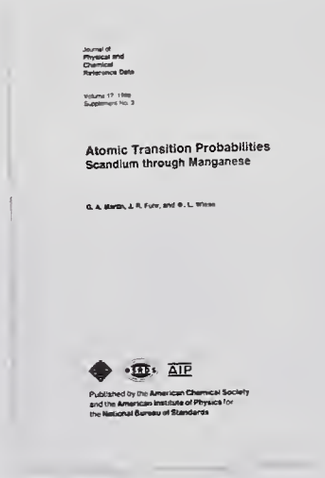


Jeff Fuhr (l) and Dr. Wolfgang Wiese of the Atomic Transition Probabilities Data Center measure intensities of spectral lines with a wall-stabilized arc.

ATOMIC PHYSICS PUBLICATIONS

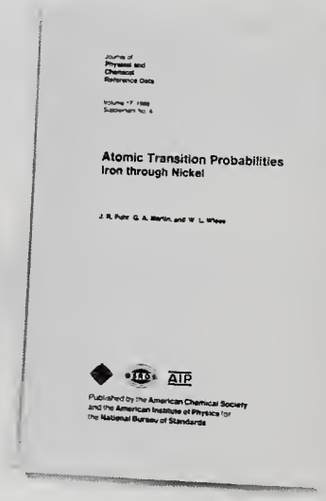
Atomic Transition Probabilities, Scandium Through Manganese—G.A. Martin, J.R. Fuhr, and W.L. Wiese. Journal of Physical and Chemical Reference Data **17**, Supplement 3, 1988.

Atomic Transition Probabilities, Iron Through Nickel—J.R. Fuhr, G.A. Martin, and W.L. Wiese. Journal of Physical and Chemical Reference Data **17**, Supplement 4, 1988.



These two supplements to the Journal of Physical and Chemical Reference Data contain almost 18,000 atomic transition probabilities. With over 1,000 pages of tables and critical discussion, it is the first comprehensive reference source for the transition probabilities of the eight transition metals, scandium through nickel. The data in these two volumes are presented by element and spectrum. Finding lists are provided to facilitate transition location. The tables include spectroscopic classification, wavelengths of the transitions, and the lower- and upper-energy levels and their statistical weights. For each line, an uncertainty estimate, the result of careful, critical evaluation, is given.

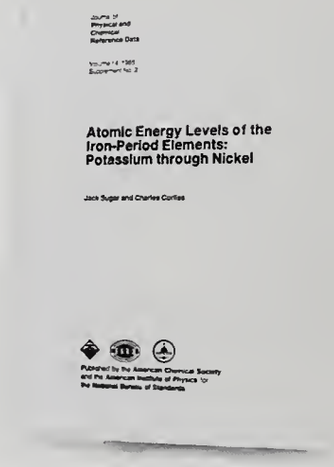
Both available from the American Chemical Society
U.S. and Canada $65.00 each
Abroad $78.00 each



Atomic Energy Levels of the Iron-Period Elements: Potassium Through Nickel—J. Sugar and C. Corliss. Journal of Physical and Chemical Reference Data **14**, Supplement 2, 1985.

This supplement is a compilation of atomic energy levels of the iron-period elements, potassium through nickel, in all stages of ionization. The result of a critical evaluation of all literature published through 1985, it gives for each energy level the position relative to the ground state, configuration, term designation, J-value, and, where available, the g-value and the two leading percentages of the eigenvector composition in the most appropriate coupling scheme. This is an invaluable research tool for atomic, molecular, plasma, and astronomical scientists.

Available from the American Chemical Society
U.S. and Canada $50.00
Abroad $58.00



Energy Levels of Phosphorus, P I through P XV—W.C. Martin, R. Zalubas, and A. Musgrove. Journal of Physical and Chemical Reference Data **14**, 751 (1985).

Energy levels data are given for the atom and all positive ions of phosphorus (Z=15). These data have been critically compiled, mainly from published and unpublished material on measurements and analyses of the optical spectra. The levels for a number of the ions have been derived or recalculated. In addition to the level values in cm^{-1} and the parity, the J value and the configuration and term assignments are listed if known. Leading percentages from the calculated eigenvectors are tabulated or quoted wherever available. Ionization energies are given for all spectra.
Available from the American Chemical Society, Reprint 278, $8.00

Dr. William C. Martin, Director (l), Dr. Jack Sugar, and Ms. Arlene Musgrove of the Atomic Energy Levels Data Center review energy level data.

Spectral Data for Molybdenum Ions, Mo VI - Mo XLII—Toshizo Shirai, Yohta Nakta, Kunio Ozawa, Keishi Ishii, Jack Sugar, and Kazuo Mori. Journal of Physical and Chemical Reference Data **16**, 327 (1987).

Wavelengths, intensities, and classifications for molybdenum ions are compiled. A short review of the work on each stage of ionization is included. The data have been critically evaluated and the best results are quoted.
Available from the American Chemical Society, Reprint 324, $8.00

Energy Levels of Molybdenum, Mo I through Mo XLII—Jack Sugar and Arlene Musgrove. Journal of Physical and Chemical Reference Data **17**, 155 (1988).

The energy levels of the molybdenum atom, in all stages of ionization for which experimental data are available, have been compiled. Ionization energies, either experimental or theoretical, have experimental g-factors given. Leading components of calculated eigenvectors are listed.
Available from the American Chemical Society, Reprint 340, $10.00

Wavelengths and Energy Level Classifications of Scandium Spectra for All Stages of Ionization—V. Kaufman and J. Sugar. Journal of Physical and Chemical Reference Data **17**, 1679 (1988).

Wavelengths and their classifications are compiled for the spectra of scandium, Sc I through Sc XXI. Selections of data are based on the critical evaluations in the compilation of energy levels by Sugar and Corliss. These are updated by a thorough search of the subsequent literature. All classifications are verified with predictions made by differencing the energy levels. Spectra are ordered by ionization stage and listed by wavelength. Two finding lists are included.
Available from the American Chemical Society, Reprint 352, $11.00

Collisional Alignment and Orientation of Atomic Outer Shells I. Direct Excitation by Electron and Atom Impact—Nils Andersen, Jean W. Gallagher, and Ingolf V. Hertel. Physics Reports **165**, July 1988.

Data describing the dynamics of the excited state charge cloud resulting from low-energy electron or ion impact on atomic targets are reviewed. Various research groups have used different parameterizations to express these data acquired from observation of the polarization of radiation emitted following excitation. In this review, all data are reformatted into a physically meaningful set of parameters which quantify the shape and angular momentum of the excited state charge cloud. The results of similar measurements by different groups are compared, and fundamental theories are tested by comparing their predictions of the same quantities. Thus, this work organizes and summarizes the field of collisional alignment and orientation of atomic outer shells by direct excitation, including all data reported prior to mid-1988, and provides a foundation for future research.
Available from Elsevier Science Publishers, $65.00

Multiphoton Bibliography 1983-1986—S.J. Smith, J.H. Eberly, J.W. Gallagher, editors. NBS-LP-**92**, Supplement 5, June 1989.

This bibliography expands the collection of references describing studies of the interaction of more than one photon with individual atoms and molecules in the gas phase. Over 1200 papers are included and classified into the categories of ionization, bound-bound, and dissociation by two-photons, three-photons, and more than three photons. The papers are also indexed by target material.
Available from JILA Data Center, University of Colorado, Boulder, CO

The 1986 CODATA Recommended Values of the Fundamental Physical Constants—E. Richard Cohen and Barry N. Taylor. Journal of Physical and Chemical Reference Data **17**, 1795 (1988).

This article presents values of the basic constants and conversion factors of physics and chemistry resulting from the 1986 least-squares adjustment of the fundamental physical constants as published by the CODATA (Committee on Data for Science and Technology) Task Group on Fundamental Constants and recommended for international use by CODATA. The 1986 CODATA set of values replaces its predecessor published by the Task Group and was recommended for international use by CODATA in 1973.
Available from the American Chemical Society, Reprint 354, $5.00

Bremsstrahlung Energy Spectra from Electrons with Kinetic Energy 1 keV-10 GeV Incident on Screened Nuclei and Orbital Electrons of Neutral Atoms with Z = 1-100—Stephen M. Seltzer and Martin J. Berger. Atomic Data and Nuclear Data Tables **35**, 345 (1986).

In this publication, a comprehensive set of bremsstrahlung cross sections is tabulated. The set includes results for electrons with energies from 1 keV to 10 GeV incident on neutral atoms with atomic numbers Z = 1 to 100. A numerical interpolation scheme, applied to suitably-scaled cross sections, was used to bridge the gap between low-energy and high-energy theoretical results.
Available from Academic Press, 0092-640X/86, $3.00

X-ray Attenuation Cross Sections for Energies 100 eV to 100 keV and Elements Z = 1 to Z = 92—E.B. Saloman and J.H. Hubbell. Atomic Data and Nuclear Data Tables 38, 1 (1988).

In this work, the NIST database of experimental x-ray attenuation coefficients and cross sections for the energy range 0.1-100 keV is calculated using a relativistic Hartree-Slater model for the photoelectric cross section for all elements of atomic number Z = 1-92. The information is displayed in both tabular and graphic form. A bibliography of the NIST database for this energy range is included.
Available from Academic Press, 0092-640X/88, $3.00

Bibliography of Photon Total Cross Section (Attenuation Coefficient) Measurements 10 eV to 13.5 GeV—J.H. Hubbell, H.M. Gerstenberg, and E.B. Saloman. NBSIR 86-3461, 99 pp. (1986).

This bibliography presents papers reporting absolute measurements of photon (XUV, x-ray, gamma-ray, bremsstrahlung) total interaction cross sections or attenuation coefficients for the elements and some compounds. The energy range covered is from 10 eV to above 10 GeV.
Available from NTIS, Order No. PB 87-116141

CHEMICAL KINETICS

The NIST Program on Chemical Kinetics Data has long been a source of reliable, critically evaluated data on gas-phase reactions. Over the years, data provided by the program have been instrumental in modeling and predicting many important scientific problems such as combustion chemistry, atmospheric changes caused by ozone depletion and warming, plasmas, and free-radical chemistry.

Recently, a comprehensive, easy-to-use PC database on over 2,000 gas-phase reactions has been widely distributed allowing scientists quick access to reaction rate data, as well as supporting information. In addition, the Radiation Chemistry Data Center at Notre Dame University provides a biweekly literature current awareness service on kinetics of ions, and free-radicals.

SRD Chemical Kinetics Database

NIST Chemical Kinetics Database

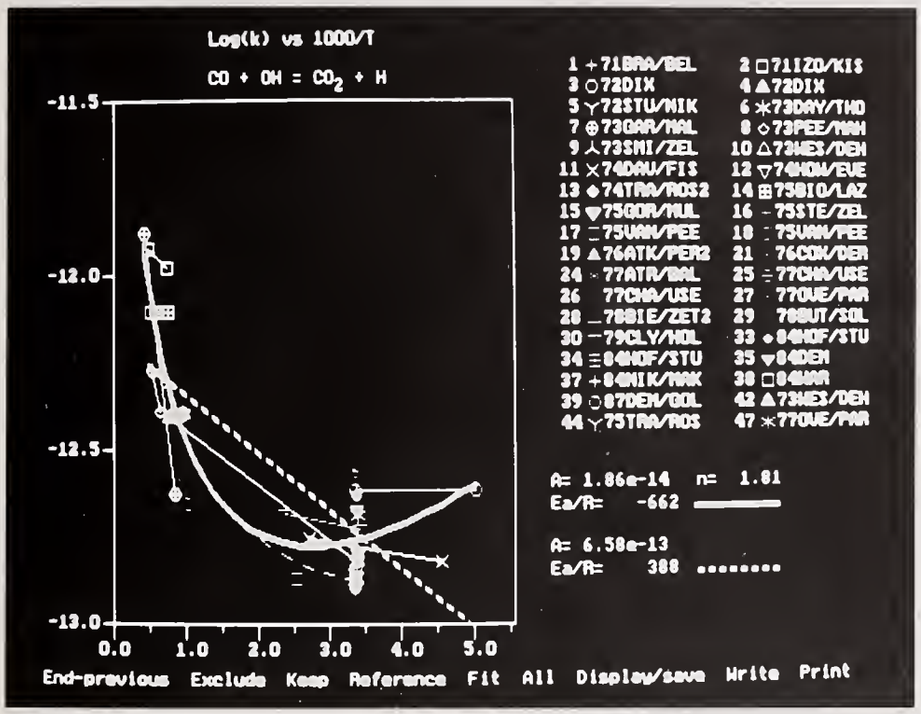
SRD Major Publications in Chemical Kinetics

Biweekly List of Papers on Radiation Chemistry and Photochemistry
Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen $O(^3P)$ with Unsaturated Hydrocarbons
Chemical Kinetic Data Base for Combustion Chemistry. Part 2. Methanol
Chemical Kinetic Data Base for Combustion Chemistry. Part 3. Propane

CHEMICAL KINETICS DATABASE

17. NIST Chemical Kinetics Database

W. Gary Mallard
Chemical Kinetics Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301)975-2564



An Arrhenius graph of a rate constant in the NIST Chemical Kinetics Database.

The NIST Chemical Kinetics Database is designed to provide rapid access to kinetics data for gas-phase reactions including surveys of the literature on a particular reaction, all of the reactions of a given species, subsets of all of the reactions, and the data available from a given paper. A highly interactive program allows users to search by reactants or by reference. The database contains more than 2,000 separate reactions and 8,000 records. The results of a search can be graphically displayed and mathematically fit to standard kinetic equations.

The database contains the following information on each rate constant record:

- Reactants and, if defined, products of the reaction
- Rate parameters: A, n, (E_a/R) where $k = A\,(T/298)^n \exp(-E_a/R)/T)$
- Uncertainty in A, n, and E_a/R if reported
- Temperature range of experiment, or temperature range of validity for a review or theoretical paper
- Pressure range and bulk gas of the experiment
- Data type of the record; i.e., direct measurement, relative rate measurement, theoretical, etc.
- Experimental procedure, including analytical procedures, excitation technique, etc.

This database is available in PC diskette format. Regular updates are planned.

Drs. W. Gary Mallard (l) and John T. Herron demonstrate the NIST Chemical Kinetics Database.

CHEMICAL KINETICS PUBLICATIONS

Biweekly List of Papers on Radiation Chemistry and Photochemistry—Radiation Chemistry Data Center, Notre Dame, IN.

This is a current-awareness publication with special emphasis on the kinetics and other properties of transient ions, radicals, and excited species in solution. Papers are included on the radiation chemistry and photochemistry of chemically-defined systems containing organic and inorganic compounds, biological molecules, and polymers, with references to ESR and luminescence studies. The references listed are obtained from scanning 60 current journals, as well as Chemical Abstracts, INIS Atomindex, and other publications.
Available from the Radiation Chemistry Data Center, Radiation Laboratory, University of Notre Dame

Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen $O(^3P)$ with Unsaturated Hydrocarbons—R.J. Cvetanovic. Journal of Physical and Chemical Reference Data **16**, 261 (1987).

Chemical kinetic data for reactions of $O(^3P)$ atoms with unsaturated hydrocarbons are compiled and critically evaluated. Interactions with alkenes, cycloalkenes, halogen-substituted alkenes and ketenes, alkynes, halogen-substituted alkynes, aromatic hydrocarbons, halogen-substituted aromatic hydrocarbons, and pyridines are included. All kinetic data considered were restricted to gas-phase reactions.
Available from the American Chemical Society, Reprint 323, $9.00

Chemical Kinetic Data Base for Combustion Chemistry. Part 2. Methanol—Wing Tsang. Journal of Physical and Chemical Reference Data **16**, 471 (1987).

This publication contains evaluated and estimated data on the kinetics of reactions involving methanol and hydroxymethyl radicals and various small inorganic and organic species which are of importance for methanol combustion and pyrolysis.
Available from the American Chemical Society, Reprint 327, $7.00

Chemical Kinetic Data Base for Combustion Chemistry. Part 3. Propane—Wing Tsang. Journal of Physical and Chemical Reference Data **17**, 887 (1988).

With evaluated and estimated data on the kinetics of reactions involving propane, isopropyl radical, n-propyl radical, and various small inorganic and organic species, this publication is important for propane pyrolysis and combustion.
Available from the American Chemical Society, Reprint 344, $9.00

MATERIALS PROPERTIES

The NIST Materials Data Program concentrates on providing evaluated data in three areas: phase equilibria, structure and characterization, and performance properties. Phase equilibrium data are addressed in two large cooperative programs. The NIST/ASM Alloy Phase Diagram Program has systematically evaluated all binary alloy phase diagrams. The NIST/American Ceramics Society Program for Phase Diagrams for Ceramists is now working on its ninth volume.

Crystallographic, electron diffraction, and surface analysis data form the bulk of the Structure and Characterization Program, and databases are available in all three areas. The databases are discussed in more detail under Analytical Chemistry. Corrosion and tribology performance data are also cooperative activities, in conjunction with the National Association of Corrosion Engineers and ACTIS, Inc., respectively, and several databases produced by these programs have gained wide acceptance.

SRD Materials Properties Databases

COR*SUR1—corrosion rate data for metals
COR*SUR2—corrosion rate data for nonmetals
COR*DATA —corrosion database management

SRD Major Publications in Materials Properties

Bulletin of Alloy Phase Diagrams
Phase Diagrams for Ceramists

MATERIALS PROPERTIES DATABASE

16. NACE-NIST Corrosion Performance Database

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(301)975-6026

Three corrosion databases developed under the NACE-NIST Corrosion Data Program give users reference data for general guidance on the performance of engineering materials in corrosive environments. COR*SUR1 includes data for 25 common metals for exposures in over 1,000 corrosive environments at various temperatures and concentrations. COR*SUR2 provides similar data for 36 nonmetallic materials (elastomers, polymers, composites, thermoplastics, etc.) in over 850 environments. Data can be retrieved from both programs by:

- tabular listing of materials exhibiting a specified range of corrosion rates in selected environments
- graphic presentation of corrosion rate ranges for a given material in a matrix of environment, concentration, and temperature
- tabular listing of corrosion rate data for a specified material in a corrosive environment as a function of temperature and concentration

Dr. David B. Anderson and Carole Derr Flanigan of the Corrosion Data Center.

The COR*DATA Corrosion Database Management System provides PC-based capability to corrosion scientists and engineers.

Programs are derived from Corrosion Data Survey publications produced by the National Association of Corrosion Engineers (NACE) and are available in diskette form for use on IBM or compatible personal computer systems from NACE, P.O. Box 218340, Houston, TX 77218.

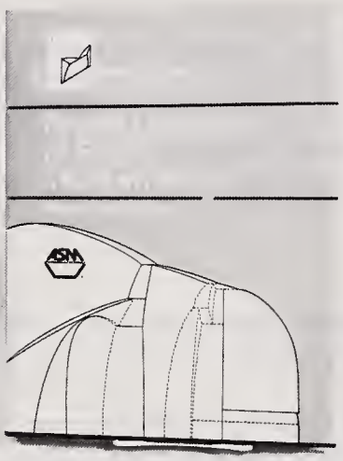
MATERIALS PROPERTIES PUBLICATIONS

Bulletin of Alloy Phase Diagrams—ASM International, Metals Park, OH.

This bimonthly publication features binary, ternary, and higher-order phase diagrams and provides tear-out diagrams. Evaluated by international experts, these diagrams are invaluable predictive and interpretive tools in determining the properties of combinations of metals.
Available from ASM International, Metals Park, OH

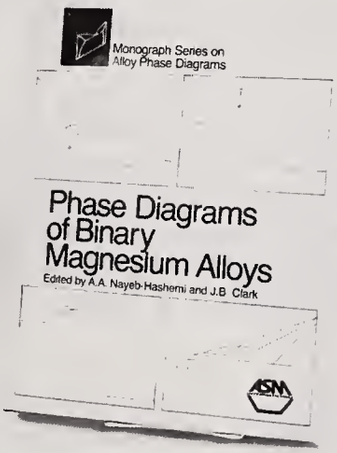
Phase Diagrams of Binary Titanium Alloys—edited by Joanne L. Murray, ASM International, Metals Park, OH.

The most complete source of data for all binary titanium systems, this volume has 66 illustrations, including 60 phase diagrams. The crystal structure and lattice parameter tables are included, along with a bibliography, through the end of 1985.
Available from ASM International, Metals Park, OH



Phase Diagrams of Binary Magnesium Alloys—edited by A.A. Nayeb-Hashemi, ASM International, Metals Park, OH.

This volume evaluates pure magnesium plus 78 binary magnesium alloys. With 106 illustrations, including 61 phase diagrams, this reference source details crystal structures and lattice parameter tables. A complete bibliography is included through the end of 1986.
Available from ASM International, Metals Park, OH



Phase Diagrams of Binary Vanadium Alloys—edited by Jack L. Smith, ASM International, Metals Park, OH.

Evaluating pure vanadium plus 79 binary vanadium alloys, this is the most complete source of data for vanadium. This volume includes 125 illustrations with 50 phase diagrams and the crystal structure and lattice parameter tables. A bibliography through mid-1988 is another feature.
Available from ASM International, Metals Park, OH

Thermodynamic Properties of Iron and Silicon—P.D. Desai. Journal of Physical and Chemical Reference Data **15**, 967 (1986).

This work reviews the data on the various thermodynamic properties of iron and silicon through 1984. The properties include heat capacity, enthalpy, enthalpies of transition and melting, vapor pressure, and enthalpy of vaporization. The recommended values for heat capacity, enthalpy, entropy, and Gibbs energy function cover the energy range from 1 to 3200 K for iron and 1 to 3600 K for silicon. The recommended values for vapor pressure cover the temperature range from 298.15 to 3200 K for iron and from 298.15 to 3600 K for silicon.
Available from the American Chemical Society, Reprint 298, $6.00

Phase Diagrams and Thermodynamic Properties of the 70 Binary Alkali Halide Systems Having Common Ions—James Sangster and Arthur D. Pelton. Journal of Physical and Chemical Reference Data **16**, 509 (1987).

This work is a very extensive literature survey of all available phase diagram and thermodynamic data for all 40 possible common-anion binary systems (AX-BX) and all 30 possible common-cation binary systems (AX-AY) involving the alkali halides. A computer-assisted coupled analysis of the phase diagram data and the thermodynamic data for each system has been employed. Mathematical expressions for the thermodynamic properties of all known phases have been obtained which are consistent with the measured thermodynamic properties and phase diagrams, as well as with established thermodynamic principles and theories of solution behavior.
Available from the American Chemical Society, Reprint 330, $8.00

Critical Compilation of Surface Structures Determined by Low-Energy Electron Diffraction Crystallography—Philip R. Watson. Journal of Physical and Chemical Reference Data **16**, 953 (1987).

This review critically compiles all surface structures derived from low-energy electron diffraction (LEED) crystallography reported in the referenced literature. Over 250 investigations covering all types of surfaces including clean and adsorbate-covered metal, semiconductor, and other nonmetallic substrates have been analyzed. Objective criteria have been applied to the estimation of the reliability of a particular structural determination. This compilation will provide a valuable resource both for the surface science specialist and for the nonspecialist in other areas who need surface crystallographic data.
Available from the American Chemical Society, Reprint 336, $7.00

Phase Diagrams for Ceramists—American Ceramic Society, Columbus, OH.

This publication series has become the definitive source of ceramic phase diagrams in the scientific community. These nine volumes contain commentaries and binary, ternary, and higher-order phase diagrams of oxide, metals-oxide, and metal-oxygen systems, halide, and other ceramic systems.
Available from the American Ceramic Society, Columbus, OH

MOLECULAR STRUCTURE AND SPECTROSCOPY

Building upon the renowned NIST research on molecular structure, the SRD Program has produced several important compilations of molecular data. Numerous comprehensive microwave spectra for astrophysically interesting molecules have been published and are widely used in radio astronomy. In addition, several comprehensive compilations of microwave spectral tables are now available.

A new database on vibrational and electronic lines has been prepared and will be updated yearly.

SRD Molecular Structure and Spectroscopy Database

NIST Vibrational and Electronic Energy Levels of Small Polyatomic Molecules

MOLECULAR STRUCTURE AND SPECTROSCOPY DATABASE

26. NIST Vibrational and Electronic Energy Levels of Small Polyatomic Molecules

Marilyn Jacox
National Institute of Standards and Technology
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(301)975-2547

This database is designed to give rapid access to experimental data on ground-state vibrational fundamentals, the electronic energy levels, and the vibrational fundamentals of transient molecules with from 3 to 6 atoms in their excited electronic states. Data on approximately 1,000 molecules are included. Searches can be conducted by molecule or wavenumber or, for electronic band origins, by wavelength range in which the transition appears. Searches can be restricted to molecules containing a specified chemical element, to either the ground or excited electronic states, to observations in the gas-phase or in a specified inert solid matrix, or to data obtained using a specific technique. Provision is made for the display of references to the original literature pertinent to each line of the compilation or of all references associated with the molecule of interest.

This database is available in PC diskette format.

MOLECULAR STRUCTURE AND SPECTROSCOPY PUBLICATIONS

Microwave Spectra of Molecules of Astrophysical Interest. XXI. Ethanol (C_2H_5OH) and Propionitrile(C_2H_5CN) — F.J. Lovas. Journal of Physical and Chemical Reference Data 11, 251 (1982).

The microwave spectra of ethanol and propionitrile are critically reviewed and supplemented with spectral frequency calculations which include rotational and centrifugal distortion terms in the molecular Hamiltonian. This review provides the microwave transition frequencies applicable to molecular radio astronomy for the ground vibrational state of the most abundant isotopic forms.
Available from the American Chemical Society, Reprint 201, $8.00

Frank J. Lovas and Gloria Rotter of the Molecular Spectra Data Center verify data used in their compilations.

Microwave Spectra of Molecules of Astrophysical Interest. XXII. Sulfur Dioxide (SO_2)—F.J. Lovas. Journal of Physical and Chemical Reference Data **14**, 395 (1985).

The microwave spectrum of sulfur dioxide (SO_2) is critically reviewed and supplemented with spectral frequency calculations derived from rotational and centrifugal distortion terms in the molecular Hamiltonian. This review provides the microwave transition frequencies applicable to molecular radio astronomy for the ground vibrational states of the most abundant isotopic forms, the singly substituted atoms ^{33}S and ^{34}S.
Available from the American Chemical Society, Reprint 271, $10.00

Microwave Spectral Tables III. Hydrocarbons, CH to $C_{10}H_{10}$—F.J. Lovas and R.D. Suenram. Journal of Physical and Chemical Reference Data **18**, 1245 (1989).

All of the rotational spectral lines observed and reported in the open literature for 91 hydrocarbon molecules have been tabulated. The isotopic molecular species, assigned quantum numbers, observed frequency, estimated measurement uncertainty, and references are given for each transition reported. The derived molecular properties, such as rotational and centrifugal distortion constants, hyperfine structure constants, electric dipole moments, and rotational g-factors, are listed.
Available from the American Chemical Society, Reprint 369, $22.00

Triplet-Triplet Absorption Spectra of Organic Molecules in Condensed Phases—Ian Carmichael and Gordon L. Hug. Journal of Physical and Chemical Reference Data **15**, 1 (1986).

This is a compilation of spectral parameters associated with triplet-triplet absorption of organic molecules in condensed media. The wavelengths of maximum absorbance and extinction coefficients have been critically evaluated. The triplet state process in solution and solids is presented with an historical perspective on detection and measurement. Additionally, compound name, molecular formula, and author indexes are provided.
Available from the American Chemical Society, Reprint 288, $20.00

Ground-State Vibrational Energy Levels of Polyatomic Transient Molecules—Marilyn E. Jacox. Journal of Physical and Chemical Reference Data **13**, 945 (1984).

The experimentally determined ground-state vibrational energy levels of approximately 480 covalently bonded transient molecules possessing from 3 to 16 atoms are tabulated, together with references to the pertinent literature. The types of measurement surveyed include laser-based high resolution gas- phase infrared absorption and visible-ultraviolet photoelectron spectroscopy, and matrix isolation spectroscopy.
Available from the American Chemical Society, Reprint 257, $12.00

Electronic Energy Levels of Small Polyatomic Transient Molecules—Marilyn E. Jacox. Journal of Physical and Chemical Reference Data **17**, 269 (1988).

The experimentally determined electronic energy levels of approximately 500 neutral and ionic transient molecules possessing from 3 to 6 atoms are tabulated, together with the associated vibrational structure, the radiative lifetime, the principal rotational constants, and references to the present literature. Vibrational and rotational data for the ground state are also given. Observations in the gas-phase, in molecular beams, and in rare-gas and nitrogen matrices are included.
Available from the American Chemical Society, Reprint 342, $20.00

THERMOCHEMISTRY

NIST has a long history as the source for reliable thermochemical data starting with the International Critical Tables from the 1920's. The tradition continues as new SRD databases on thermochemical properties of inorganic and small organic molecules gain acceptance. The NIST Standard State Thermochemical Tables are recognized as the internationally authoritative source of these data. The JANAF Thermochemical Tables contain the most complete compilations of evaluation temperature thermodynamic data for inorganic species.

Specialized collections of data for water and aqueous electrolytes complement the standard collections. In addition, a number of detailed collections on specific families of organic and inorganic compounds are available. NIST thermochemical databases are available both in convenient PC formats and as online systems.

SRD Thermochemical Databases

NIST Chemical Thermodynamics Database
NIST Thermophysical Properties of Water Database
NIST JANAF Thermochemical Tables
NIST Activity and Osmotic Coefficients of Aqueous Electrolyte Solutions
DIPPR Data Compilation of Pure Compound Properties
NIST Positive Ion Energetics Database
NIST Negative Ion Energetics Database

SRD Major Publications in Thermochemistry

NBS Tables of Chemical Thermodynamic Properties
JANAF Thermochemical Tables
NBS/NRC Steam Tables

2. NIST Chemical Thermodynamics Database

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This database contains recommended values for selected thermodynamic properties of more than 15,000 inorganic substances. These properties include the following:

Standard state properties at 298.15 K and 1 bar
- enthalpy of formation from the elements in their standard state
- Gibbs (free) energy of formation from the elements in their standard state
- entropy
- enthalpy $H°(298.15\ K) - H°(0\ K)$
- heat capacity at constant pressure

Properties at 0 K
- enthalpy of formation

The database is not presently supplied with search software, but a PC Version is currently in preparation. It is available in a magnetic tape format and online through STN and CIS.

10. NIST Thermophysical Properties of Water

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National Institute of Standards and Technology
Gaithersburg, MD 20899
(301)975-2455

This database consists of an interactive program which calculates the thermodynamic properties of fluid H_2O (liquid and vapor) using the formulation as approved by the International Association for the Properties of Steam (IAPS) at its Tenth International Conference in 1984.

The interactive FORTRAN 77 program consists of three parts. The first part contains a package of subroutines to calculate the thermodynamic and transport properties of fluid H_2O. The other parts are main programs which call these routines to generate properties of H_2O interactively.

The first main program allows the calculation and display of all properties at a single pair of independent variables:

pressure – temperature

density – temperature

entropy – temperature

enthalpy – temperature

enthalpy – pressure

The second main program allows the generation of tables of properties along isotherms, isobars, or isochores. To keep the tabular form compact, the user may choose which properties are to be displayed.

The range approved by IAPS for this formulation includes temperatures from 0 to 1000° C and pressures up to 1500 MPa. The range over which usable results will be obtained extends to 2500 K and to 3000 MPa.

The printed version of this database, which includes a description of the data selection and evaluation procedures, is found in NBS/NRC Steam Tables-L. Haar, J. S. Gallagher, and G. S. Kell. Hemisphere Press, Washington, DC, 1984.

13. NIST JANAF Thermochemical Tables

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National Institute of Standards and Technology
Standard Reference Data
Gaithersburg, MD 20899
(301)975-2200

The JANAF Thermochemical Tables provide a compilation of critically evaluated thermodynamic properties of approximately 1800 substances over a wide range of temperatures. Recommended temperature-dependent values are provided for inorganic substances and for organic substances containing only one or two carbon atoms.

These tables cover the thermodynamic properties with single-phase and multiphase tables for the crystal, liquid, and ideal gas states. The properties tabulated are heat capacity, entropy, Gibbs energy function, enthalpy, enthalpy of formation, Gibbs energy of formation, and the logarithm of the equilibrium constant for formation of each compound from the elements in their standard reference states. This database is consistent with the Third Edition of the JANAF Thermochemical Tables published as Supplement No. 1 to Volume 14 of the Journal of Physical and Chemical Reference Data.

This database is currently available as a magnetic tape with a PC product in preparation.

9. NIST Activity and Osmotic Coefficients of Aqueous Electrolyte Solutions

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Chemical Thermodynamics Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
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This database (called GAMPHI) provides values of activity and osmotic coefficients of binary aqueous electrolyte solutions at 298.15 K together with a collection of subroutines for utilizing this database. These thermodynamic properties are needed when performing equilibrium calculations on aqueous solutions.

Each binary electrolyte solution contains the name of the cation and anion in the binary salt; the literature reference from which the data were obtained; the minimum and maximum molality for which the data are valid; a designation of an internal database name to which the data set belongs; a designation as to whether or not the data are considered to be primary or nonprimary for a given salt in the entire database; an integer which indicates which equation or model is used to calculate the value of activity and osmotic coefficients; and the number of parameters in the model and the parameters of the model.

This database is available in magnetic tape format.

11. DIPPR Data Compilation of Pure Compound Properties

T.E. Daubert and R.P. Danner
Penn State University
133 Fenske Laboratory
University Park, PA 16802

The DIPPR database contains data on 39 properties for 1,117 chemical compounds. These data were released for public distribution by the Design Institute for Physical Property Data (DIPPR) in November 1984. Thermodynamic, physical, transport, and environmental property data are given for pure chemical compounds of high industrial priority. The database was prepared by Pennsylvania State University for the Design Institute for Physical Property Data, a cooperative project sponsored by 50 major chemical manufacturers and related companies under the auspices of the American Institute of Chemical Engineers.

For each chemical compound included, values are given for 26 single-valued property constants and for 13 properties as functions of temperature, calculated for correlation coefficients. The database also includes estimates of the accuracy of each property value and references to the sources of measured or predicted data which were used in selecting the recommended values. The database includes numeric values, as well as interactive software which allows access to specific properties of the compounds included, in any specified set of units.

This database is available in magnetic tape and diskette format.

11A. DIPPR Compilation Access Program II - Student DIPPR

This is the student version of NIST Standard Reference Database 11-DIPPR Data Compilation of Pure Compound Properties. The student version contains 100 compounds. For each compound, values are given for 26 single-valued property constants and for 13 properties as functions of temperature. The user can construct a list of compounds of interest from the available database, select any unit system, select the type of output device, and then plot or tabulate the properties of interest. An invaluable teaching tool, this database is available in diskette and magnetic tape format.

19A. NIST Positive Ion Energetics Database

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Ion Energetics Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301)975-2562

This database provides rapid access to evaluated ionization potentials, heat of formation of ions, heats of formation of the corresponding neutral species, and all references to these data. The initial source of the database is the positive ion table in "Gas-Phase Ion and Neutral Thermochemistry," Journal of Physical and Chemical Reference Data, Volume 17, Supplement 1, 1988. Evaluated proton affinity values can also be retrieved. The database has a highly interactive program that allows the user to retrieve data through three different search options: by empirical formula, by name, and by proton affinity.

Dr. Sharon G. Lias (standing) and Rhoda D. Levin review records in the NIST Positive Ion Database.

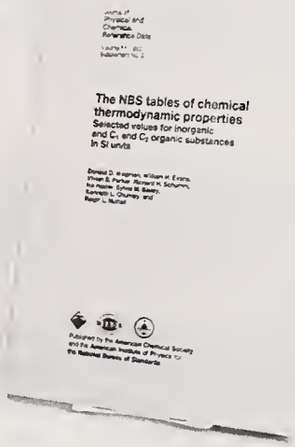
19B. NIST Negative Ion Energetics Database

John E. Bartmess
University of Tennessee
Knoxville, TN 37996

Providing immediate access to gas-phase electron affinities, acidities, negative-ion affinities to neutral species, negative-ion enthalpies of formation, and the literature references for the primary sources of the data, this database includes data on 2,000 negative ions. The species covered include all organic and inorganic atoms, molecules, and radicals for which pertinent data were found in the literature through the end of 1988. Designed to accompany the NIST Positive Ion Energetics Database, this database also uses the Journal of Physical and Chemical Reference Data, Volume 17, Supplement 1, as an initial source.

THERMOCHEMISTRY PUBLICATIONS

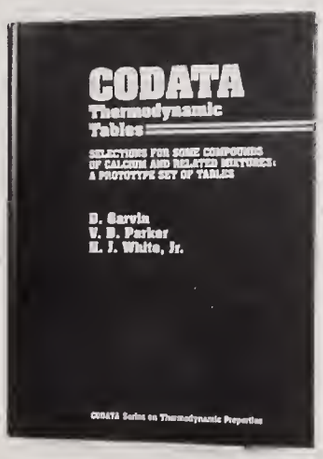
The NBS Tables of Chemical Thermodynamic Properties. II. Selected Values for Inorganic and C_1 and C_2 Organic Substances in SI Units—Donald D. Wagman, William H. Evans, Vivian B. Parker, Richard H. Schumm, Iva Halow, Sylvia M. Bailey, Kenneth L. Churney, and Ralph L. Nuttall.
Journal of Physical and Chemical Reference Data **11**, Supplement 2
(1982).



This publication provides the chemical thermodynamic properties of inorganic substances and organic substances usually containing only one or two carbon atoms. Where available, values are given for the enthalpy of formation, Gibbs energy of formation, entropy and heat capacity at 298.15 K, the enthalpy difference between 298.15 and 0 K, and the enthalpy of formation at 0 K. All values are given in SI units and are for a standard state pressure of 100,000 pascal. Gaseous, liquid, and crystalline substances, solutions in water, and mixed aqueous and organic solutions are given values. This publication supersedes the National Bureau of Standards Technical Note 270 Series.
Available from the American Chemical Society
US and Canada $40.00
Abroad $48.00

JANAF Thermochemical Tables. Third Edition—M.W. Chase, Jr., C.A. Davies, J.R. Downey, Jr., D.J. Frurip, R.A. McDonald, and A.N. Syverud. Journal of Physical and Chemical Reference Data **14**, Supplement 1 (1985).

These updated volumes contain thermodynamic properties for more than 1800 substances over a wide temperature range. All tables are in SI units and the notation has been made consistent with current international recommendations. There are single-phase and multiphase tables in the crystal, liquid, and ideal gas states. The properties tabulated are heat capacity, entropy, Gibbs energy function, enthalpy of formation, Gibbs energy of formation, and the logarithm of the equilibrium constant for formation of each compound. Each tabulation is accompanied by a critical evaluation of the literature upon which the thermochemical table is based, and literature references are given.
Available from the American Chemical Society
US and Canada $130.00
Abroad $156.00



CODATA Thermodynamic Tables. Selections for Some Compounds of Calcium and Related Mixtures: A Prototype Set of Tables—D. Garvin, V.B. Parker, and H.J. White, Jr., editors. Hemisphere, NY, 1987.

Prepared as the first of many cooperative, ongoing international projects, this volume presents recommended values for chemical thermodynamic properties of selected compounds of calcium and their mixtures. Forty-one tables of thermal functions (heat capacity, entropy, enthalpy, and Gibbs energy functions) are given for those compounds of magnesium, calcium, and potassium for which the properties have been evaluated in this work. Twenty-four tables of thermal functions are given for auxiliary substances.
Available from Hemisphere Press, ISBN 0-89116-730-7

Estimation of the Thermodynamic Properties of Hydrocarbons at 298.15 K—Eugene S. Domalski and Elizabeth D. Hearing. Journal of Physical and Chemical Reference Data **17**, 1637 (1988).

This publication extends an estimation method for calculating the thermodynamic properties of organic compounds in the gas phase to the liquid and solid phases for hydrocarbon compounds at 298.15 K. A second-order approach which includes nearest-neighbor interactions has been applied to the condensed phase. A total of 1311 comparisons are made between experimentally determined values and those calculated using additive group values. Over 140 references indicate the development of estimation methods for calculating thermodynamic properties over the last five decades.
Available from the American Chemical Society, Reprint 351, $7.00

The Thermochemical Measurements on Rubidium Compounds: A Comparison of Measured Values with Those Predicted from the NBS Tables of Chemical and Thermodynamic Properties—V.B. Parker, W.H. Evans, and R.L. Nuttall. Journal of Physical and Chemical Reference Data **16**, 7 (1987).

Illustrating the evaluation procedure used in preparing the full set of recommended data in the "NBS Tables of Chemical Thermodynamic Properties," this report presents assessed thermochemical measurements on rubidium compounds, and comparisons are made to the tables mentioned above. Estimated reliabilities on the recommended process values are given.
Available from the American Chemical Society, Reprint 311, $8.00

Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C_1 to C_4. Part 2. Ideal Gas Properties—Jing Chao, Kenneth R. Hall, Kenneth N. Marsh, and Randolph C. Wilhoit. Journal of Physical and Chemical Reference Data **15**, 1369 (1986).

The ideal gas thermodynamic properties of 44 key organic oxygen compounds in the carbon range C_1 to C_4 have been calculated by a statistical mechanical technique. Heat capacity, entropy, enthalpy, and Gibbs energy function have been determined. The thermodynamic properties have been calculated using a rigid-rotor and harmonic-oscillator molecular model for each species. The sources of molecular data and the selection of values used in the calculation are described.
Available from the American Chemical Society, Reprint 309, $9.00

NBS/NRC Steam Tables—Lester Haar, John S. Gallagher, and George S. Kell. Hemisphere Press, NY, 1984.

This landmark book presents a formulation for the properties of steam over a previously unavailable range of temperatures and pressures. Numerous thermophysical properties are tabulated, including specific volume, density, internal energy, enthalpy, and entropy. Approved by the National Institute of Standards and Technology and the International Association for the Properties of Steam and published in SI units, all physical states are calculated, including liquid, vapor, coexisting liquid/vapor, and metastables.
Available from Hemisphere Press, ISBN 0-89116-354-9 (cloth) and ISBN 0-89116-353-0 (paper)

THERMOPHYSICAL PROPERTIES OF FLUIDS

The complexity of providing reliable data on the thermochemical and thermophysical properties of fluid mixtures has been the focus of considerable attention of the SRD Program. Over the years, a set of combined theoretical and empirical predictive techniques have been developed that rest firmly on evaluated data. These techniques have been tested and incorporated into interactive computer programs that will provide a large variety of properties based upon the specified composition and the appropriate state variables.

Databases are now available for hydrocarbon mixtures, including natural gas, as well as a number of pure and mixed fluids of industrial importance.

SRD Fluids Properties Databases

NIST Thermophysical Properties of Hydrocarbon Mixtures
NIST Thermophysical Properties of Fluids
NIST Mixture Property Program
NIST Thermophysical Properties of Refrigerants and Refrigerant Mixtures

4. NIST Thermophysical Properties of Hydrocarbon Mixtures

James F. Ely
Fluid Mixtures Data Center
National Institute of Standards and Technology
Boulder, CO 80303
(303)497-3386

This database (called SUPERTRAPP) is an interactive computer program for the prediction of thermodynamic properties of mixtures which may be used for pure fluids or for mixtures of up to 20 components. The components are selected from a database of 116 components, mostly hydrocarbons. SUPERTRAPP performs phase equilibria calculations and gives the thermodynamic properties of all phases and the feed. These results include:

Equilibrium properties

- density
- compressibility factor
- enthalpy
- entropy
- *Cp*
- *Cp/Cv*
- sound speed
- Joule-Thomson coefficient

Transport properties

- viscosity
- thermal conductivity

SUPERTRAPP features commands that allow you to:

- perform bubble point pressure calculations
- perform dew point pressure calculations
- perform isothermal flash calculations
- obtain properties of pure components along the saturation boundary
- produce tables of properties along isobars or isotherms
- change units
- learn (and remember) a new component not in the current database
- enter data from the keyboard or from data files
- save results in a file

This database is available in PC diskette format.

12. NIST Thermophysical Properties of Fluids

James F. Ely
Fluid Mixtures Data Center
National Institute of Standards and Technology
Boulder, CO 80303
(303)497-3386

These interactive programs (called MIPROPS) compute thermophysical properties of 12 pure fluids: helium, argon, parahydrogen, oxygen, nitrogen, nitrogen trifluoride, ethylene, methane, ethane, propane, isobutane, and normal butane. The programs provide prompting for selection of several options including choice of fluid, choice of units, and choice of single-phase or liquid-vapor-phase calculations.

Properties are computed for the single-phase region from input of two of the following variables: temperature, pressure, and density. Values on the liquid-vapor boundary are computed for either a given temperature or a given pressure. The program returns values for pressure, temperature, density, internal energy, enthalpy, entropy, specific heats at constant volume, pressure, and sound velocity. Viscosity, thermal conductivity, and dielectric constants are given for five of the fluids.

This database is available in PC diskette and magnetic tape format.

14. NIST Mixture Property Program

James F. Ely
Fluid Mixtures Data Center
National Institute of Standards and Technology
Boulder, CO 80303
(303)497-3386

The NIST Mixture Property Program (DDMIX) is an interactive computer program which calculates various thermodynamic and transport properties of mixtures of fluids selected from any of 17 possible pure components. The emphasis of the program is on density prediction (especially for CO_2-rich mixtures), but it will provide accurate results for other properties and mixtures.

All phase equilibrium calculations are performed with the Peng-Robinson (PRS) equation of state, and coexisting phase properties are calculated with the NIST extended corresponding states model (DDMIX). Mixtures formed from any of 17 pure components (including hydrocarbons, nitrogen, oxygen, argon, carbon monoxide, carbon dioxide, and hydrogen sulfide) are handled by the program.

DDMIX provides the following outputs for any specified mixture:

- bubble point pressure
- dew point pressure
- saturation properties
- tables of density, enthalpy, entropy, and heat capacity as functions of T or P
- isothermal flash calculation yielding density, enthalpy, entropy, heat capacity, viscosity, and thermal conductivity of feed and vapor

This database is available in PC diskette format.

23. NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures

John Gallagher
Thermophysics Division
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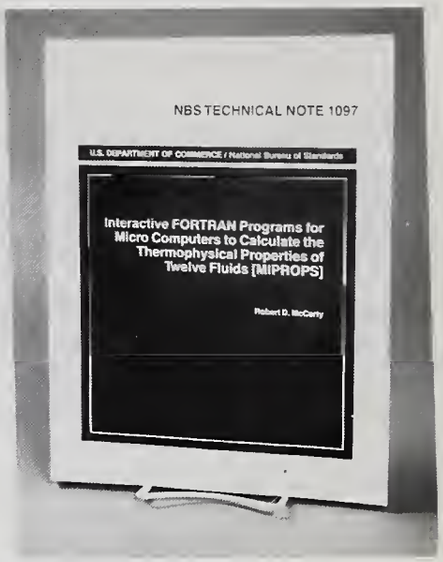
Gaithersburg, MD 20899
(301)975-2455

This database calculates the thermodynamic properties of 15 pure refrigerants and 20 binary mixtures. The package enables the user to screen several environmentally-acceptable ethane-based refrigerants and refrigerant mixtures as possible replacements for those currently used. The tables provided can be used to determine the efficiency and capability of a wide range of equipment that will be used with alternative refrigerants.

The user selects the refrigerant or refrigerant mixture of interest. REFPROP provides tables of saturation properties at desired temperatures or pressures, as well as tables of properties using any of the following as independent variables: pressure, temperature, entropy, or enthalpy. Dependent variables include those mentioned plus constant-pressure and constant-volume heat capacities and speed of sound.

THERMOPHYSICAL PROPERTIES OF FLUIDS PUBLICATIONS

Interactive FORTRAN Programs for Micro Computers to Calculate the Thermophysical Properties of Twelve Fluids—Robert D. McCarty. NBS Technical Note 1097, 84 pp. (1986).



In this publication which describes the MIPROPS database, the thermophysical and transport properties of helium, hydrogen, nitrogen, oxygen, argon, nitrogen trifluoride, methane, ethylene, ethane, propane, isobutane, and normal butane are provided. The programs detailed in this publication display properties in both the liquid and vapor states over wide ranges of temperature and pressure.
Available from Standard Reference Data, National Institute of Standards and Technology

Thermophysical Properties of Fluids. II. Methane, Ethane, Propane, Isobutane, and Normal Butane—B.A. Younglove and J.F. Ely. Journal of Physical and Chemical Reference Data **16**, 577 (1987).

Tables of thermophysical and transport properties for methane, ethane, propane, isobutane, and normal butane are presented. The mathematical relations from which these thermophysical properties are obtained are described. Pressure, density, temperature, internal energy, enthalpy, entropy, specific heat at constant pressure and at constant volume, sound speed, viscosity, thermal conductivity, and dielectric constants are listed.
Available from American Chemical Society, Reprint 331, $18.00

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